



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:15 AM UTC

PDB ID : 6OMC / pdb_00006omc
EMDB ID : EMD-20125
Title : capsid of T5 virion
Authors : Huet, A.; Duda, R.L.; Boulanger, P.; Conway, J.F.
Deposited on : 2019-04-18
Resolution : 3.80 Å(reported)
Based on initial model : 2FT1

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

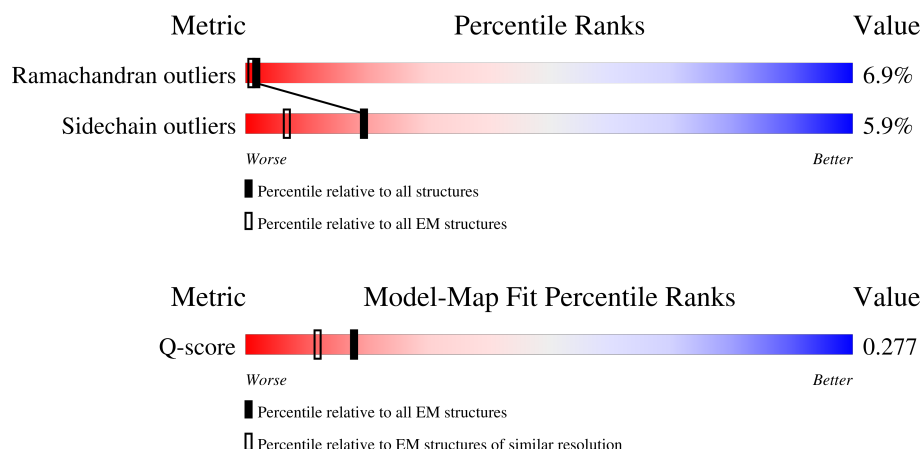
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	299	30% 84% 14% .
1	B	299	30% 83% 14% ..
1	C	299	29% 80% 17% .
1	D	299	28% 85% 12% .
1	E	299	31% 81% 17% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	299	28% 81% 16% .
1	G	299	31% 84% 14% .
1	H	299	31% 83% 14% .
1	I	299	29% 83% 15% .
1	J	299	29% 85% 13% .
1	K	299	34% 84% 14% .
1	L	299	33% 82% 16% .
1	M	299	44% 78% 18% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 60547 atoms, of which 30455 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

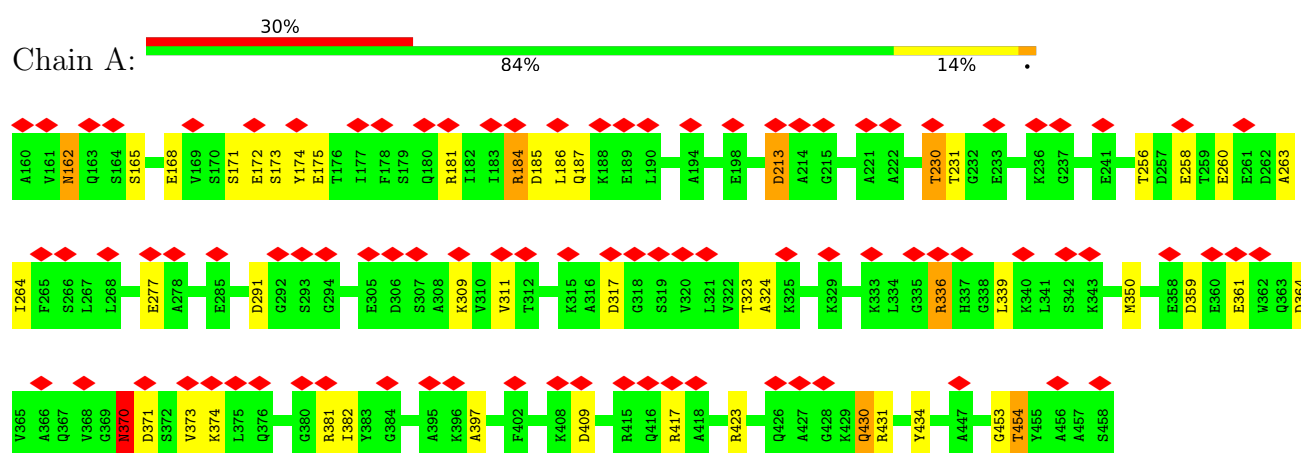
- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	B	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	C	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	D	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	E	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	F	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	G	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	H	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	I	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	J	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	K	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	L	299	Total	C	H	N	O	S	0	0
			4662	1466	2345	391	455	5		
1	M	295	Total	C	H	N	O	S	0	0
			4603	1449	2315	385	449	5		

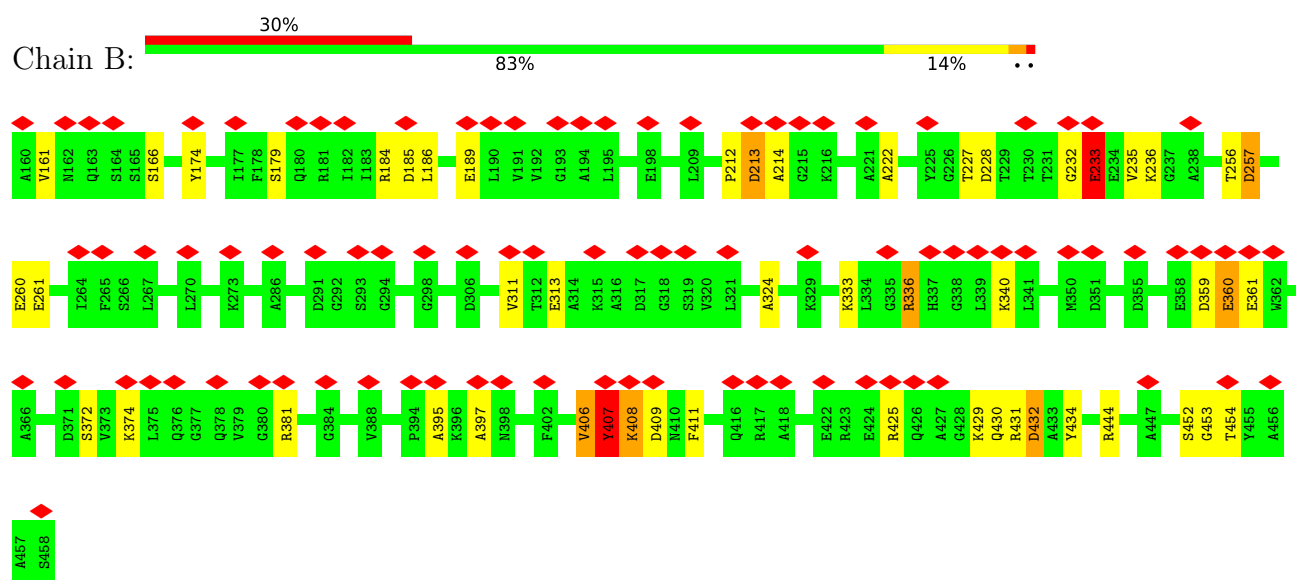
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

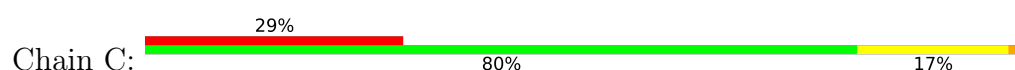
- Molecule 1: Major capsid protein

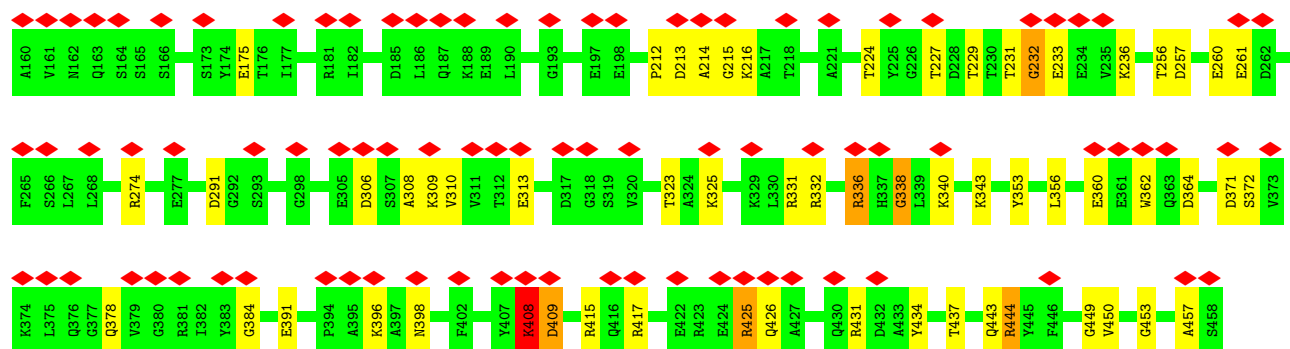


- Molecule 1: Major capsid protein

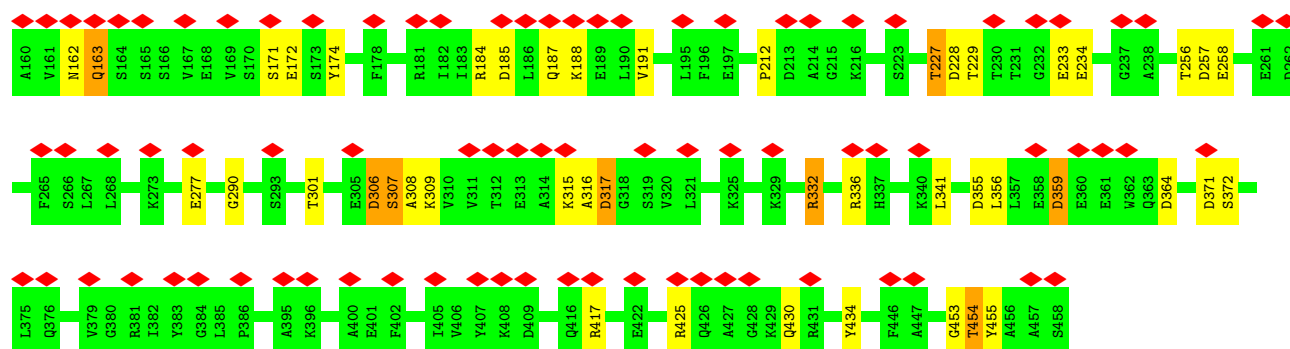
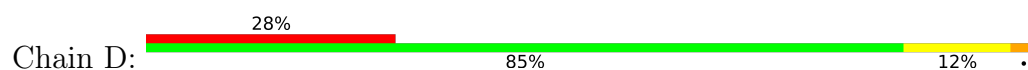


- Molecule 1: Major capsid protein

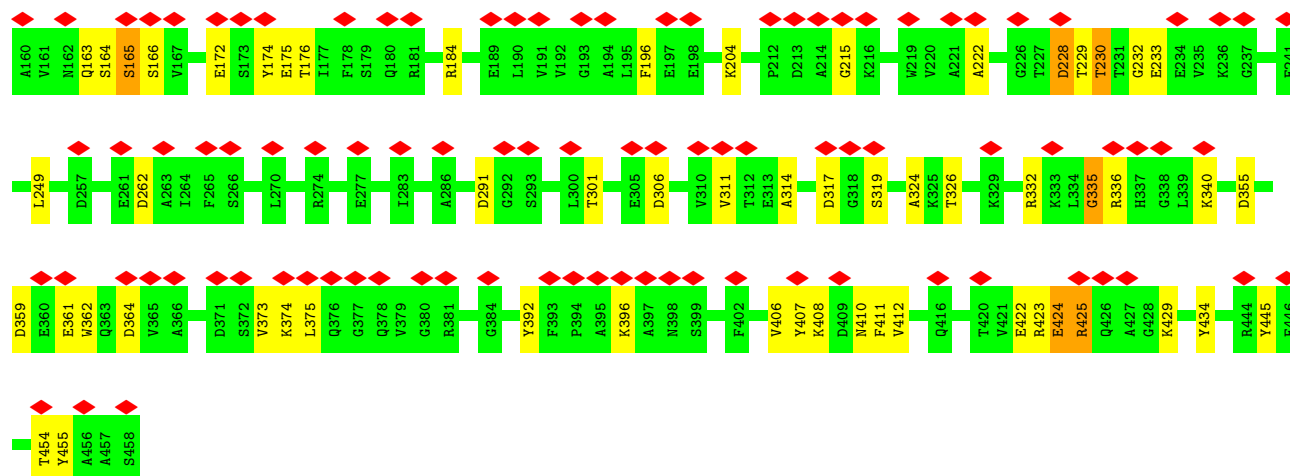
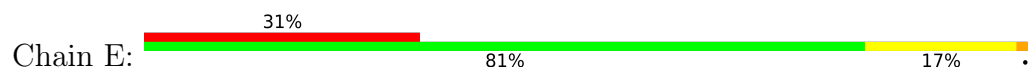




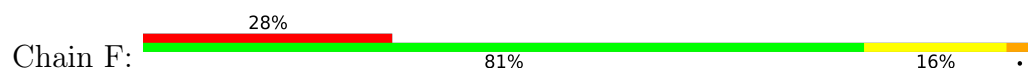
• Molecule 1: Major capsid protein

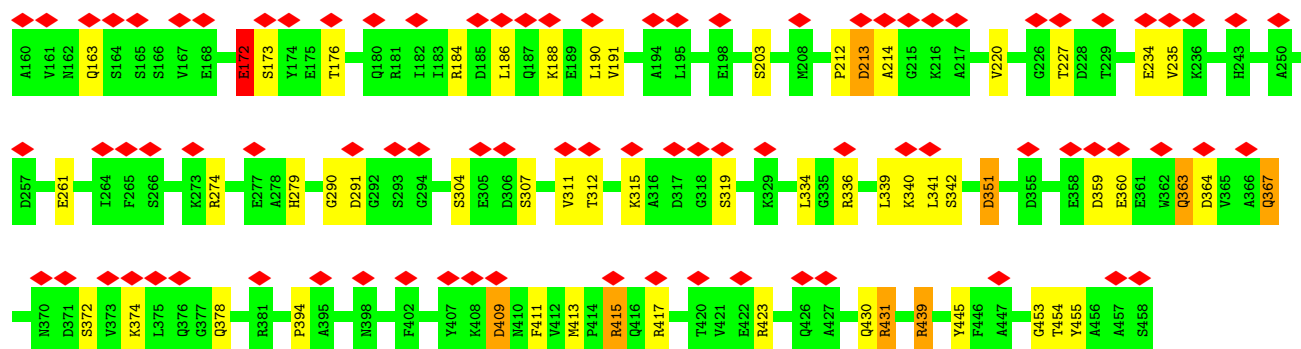


• Molecule 1: Major capsid protein

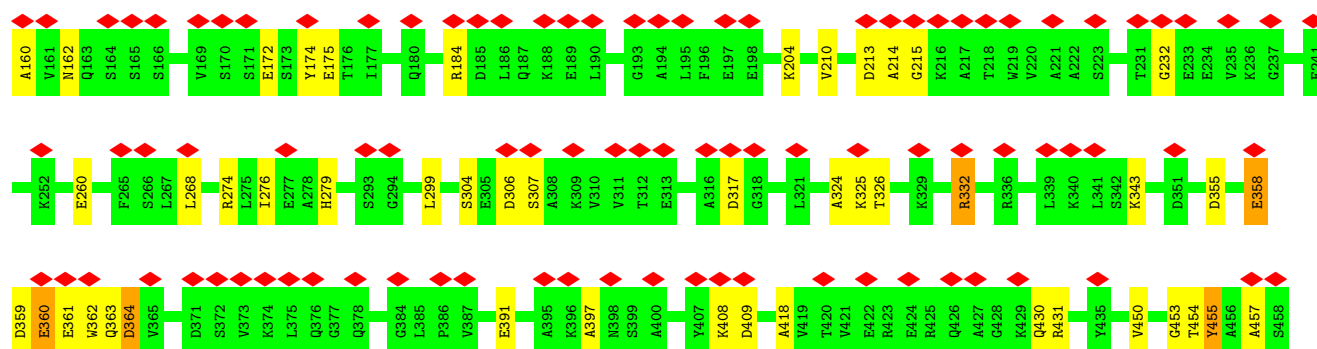
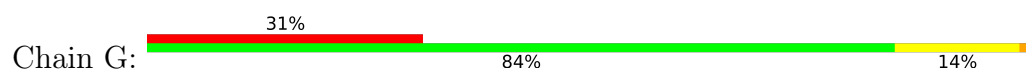


• Molecule 1: Major capsid protein

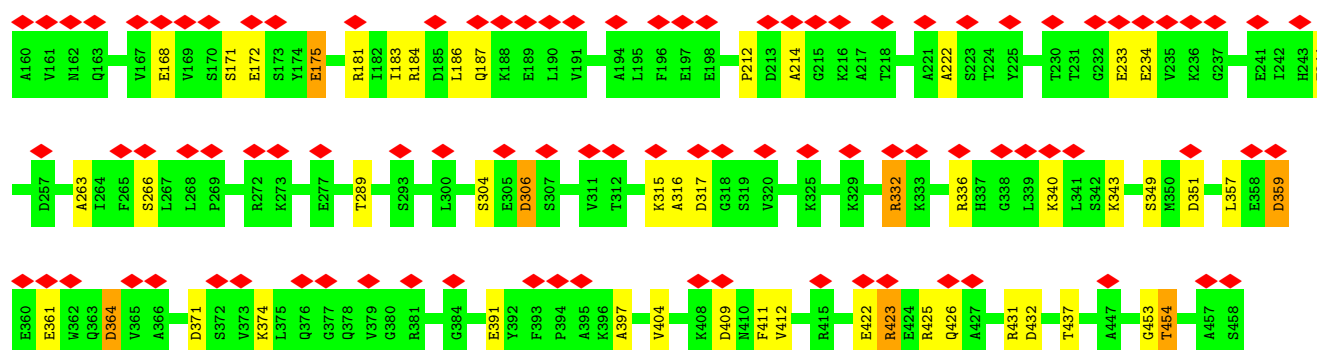
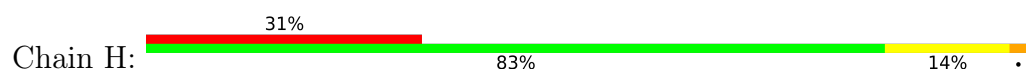




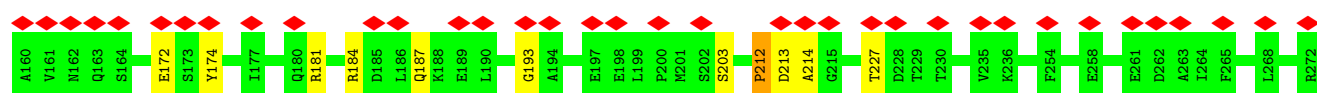
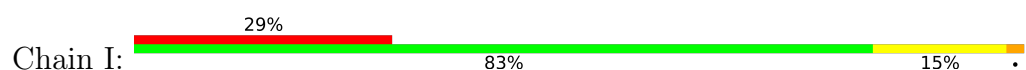
• Molecule 1: Major capsid protein

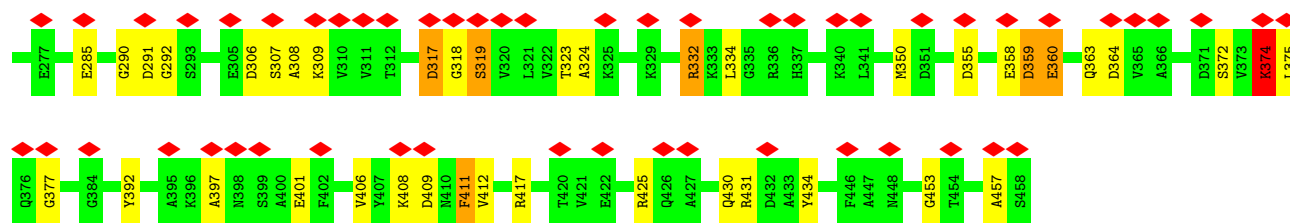


• Molecule 1: Major capsid protein

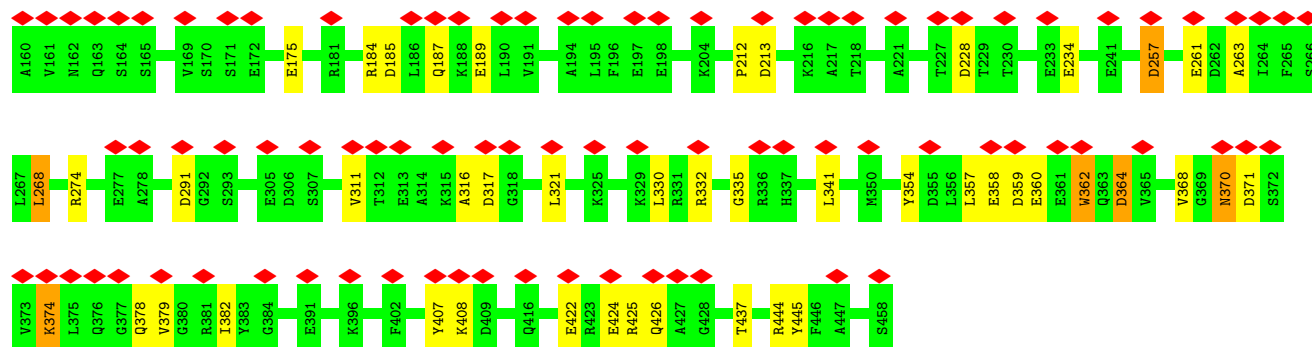
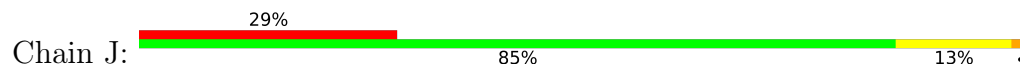


• Molecule 1: Major capsid protein

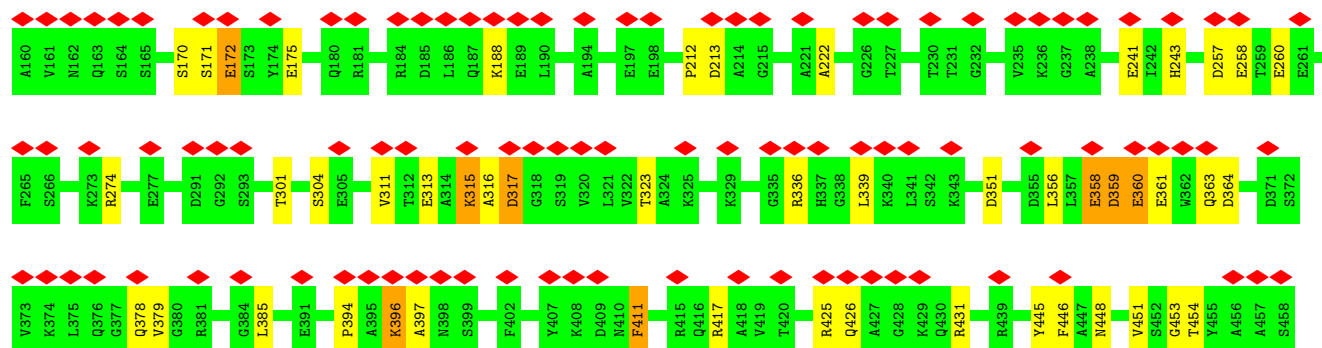
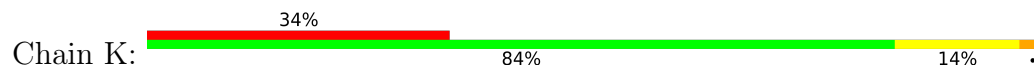




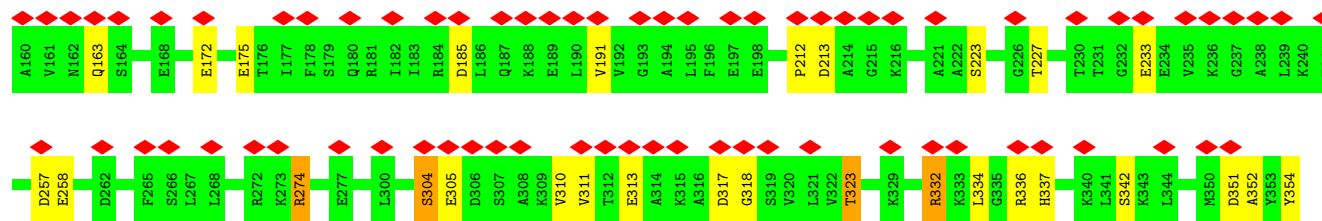
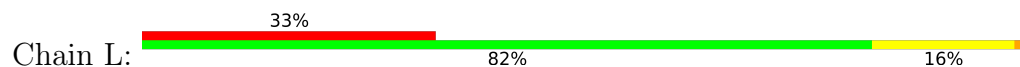
• Molecule 1: Major capsid protein

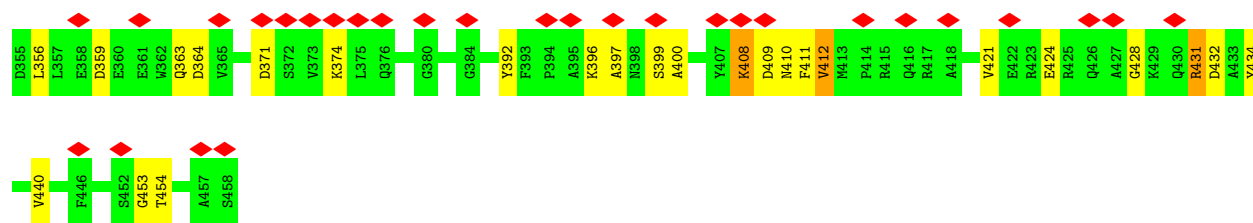


• Molecule 1: Major capsid protein

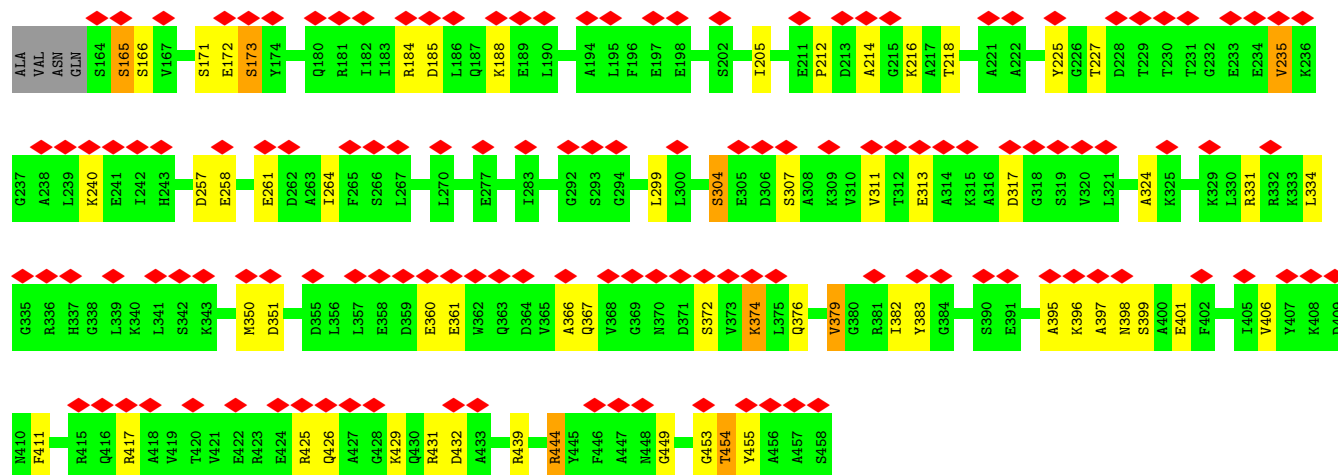
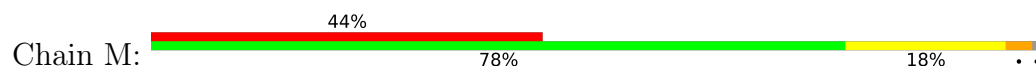


• Molecule 1: Major capsid protein





- Molecule 1: Major capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18901	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	32.443	Depositor
Minimum map value	-17.799	Depositor
Average map value	0.415	Depositor
Map value standard deviation	2.516	Depositor
Recommended contour level	8.5	Depositor
Map size (Å)	1013.85004, 1013.85004, 1013.85004	wwPDB
Map dimensions	751, 751, 751	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.90	1/2352 (0.0%)	1.61	29/3178 (0.9%)
1	B	0.88	0/2352	1.63	40/3178 (1.3%)
1	C	0.92	0/2352	1.60	23/3178 (0.7%)
1	D	0.89	0/2352	1.59	23/3178 (0.7%)
1	E	0.91	0/2352	1.64	38/3178 (1.2%)
1	F	0.89	0/2352	1.62	31/3178 (1.0%)
1	G	0.90	0/2352	1.60	26/3178 (0.8%)
1	H	0.89	0/2352	1.61	24/3178 (0.8%)
1	I	0.90	0/2352	1.59	26/3178 (0.8%)
1	J	0.90	0/2352	1.57	22/3178 (0.7%)
1	K	0.91	0/2352	1.63	32/3178 (1.0%)
1	L	0.90	0/2352	1.60	30/3178 (0.9%)
1	M	0.94	1/2323 (0.0%)	1.62	33/3138 (1.1%)
All	All	0.90	2/30547 (0.0%)	1.61	377/41274 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	6
1	C	0	12
1	D	0	6
1	E	0	9
1	F	0	9
1	G	0	6
1	H	0	5
1	I	0	9
1	J	0	5
1	K	0	5
1	L	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	5
All	All	0	93

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	383	TYR	CA-CB	5.60	1.62	1.53
1	A	184	ARG	CD-NE	5.10	1.53	1.46

All (377) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	317	ASP	CA-C-N	10.01	129.31	121.61
1	D	317	ASP	C-N-CA	10.01	129.31	121.61
1	B	359	ASP	CA-C-N	9.81	139.36	121.70
1	B	359	ASP	C-N-CA	9.81	139.36	121.70
1	J	263	ALA	CA-C-O	9.53	123.47	117.94
1	I	291	ASP	CA-CB-CG	9.01	121.61	112.60
1	L	397	ALA	CA-C-O	8.93	123.12	117.94
1	M	382	ILE	N-CA-C	8.50	120.31	110.62
1	B	408	LYS	CA-C-N	8.24	131.33	120.28
1	B	408	LYS	C-N-CA	8.24	131.33	120.28
1	B	359	ASP	CA-CB-CG	8.18	120.78	112.60
1	B	432	ASP	CA-CB-CG	8.04	120.64	112.60
1	B	359	ASP	O-C-N	-8.03	113.70	122.85
1	L	371	ASP	CA-CB-CG	7.98	120.58	112.60
1	M	454	THR	CA-C-N	7.96	136.02	121.70
1	M	454	THR	C-N-CA	7.96	136.02	121.70
1	J	359	ASP	CA-CB-CG	7.93	120.53	112.60
1	E	374	LYS	CA-C-N	7.82	135.78	121.70
1	E	374	LYS	C-N-CA	7.82	135.78	121.70
1	E	314	ALA	CA-C-O	7.75	123.21	118.33
1	E	262	ASP	CA-CB-CG	7.65	120.25	112.60
1	I	212	PRO	CA-C-N	7.65	132.34	121.02
1	I	212	PRO	C-N-CA	7.65	132.34	121.02
1	J	359	ASP	CA-C-N	7.63	135.43	121.70
1	J	359	ASP	C-N-CA	7.63	135.43	121.70
1	F	415	ARG	NE-CZ-NH1	-7.57	113.93	121.50
1	A	172	GLU	CA-C-O	7.52	122.30	117.94
1	J	359	ASP	O-C-N	-7.47	113.68	122.87
1	L	453	GLY	O-C-N	-7.47	117.82	123.35
1	A	336	ARG	O-C-N	-7.35	114.62	123.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ASN	CA-CB-CG	7.33	119.93	112.60
1	K	336	ARG	O-C-N	-7.29	114.43	123.33
1	B	212	PRO	CA-C-N	7.22	135.32	121.54
1	B	212	PRO	C-N-CA	7.22	135.32	121.54
1	C	384	GLY	CA-C-N	7.20	130.39	120.39
1	C	384	GLY	C-N-CA	7.20	130.39	120.39
1	H	374	LYS	CA-C-N	7.18	134.63	121.70
1	H	374	LYS	C-N-CA	7.18	134.63	121.70
1	F	374	LYS	CA-C-N	7.16	134.59	121.70
1	F	374	LYS	C-N-CA	7.16	134.59	121.70
1	A	317	ASP	CA-CB-CG	-7.15	105.45	112.60
1	H	263	ALA	CA-C-O	7.12	122.81	118.33
1	F	312	THR	CA-C-N	7.02	130.26	120.29
1	F	312	THR	C-N-CA	7.02	130.26	120.29
1	A	453	GLY	O-C-N	-6.99	117.37	123.80
1	E	228	ASP	CA-CB-CG	6.98	119.58	112.60
1	E	410	ASN	CA-CB-CG	6.94	119.54	112.60
1	B	360	GLU	N-CA-CB	6.94	122.30	110.50
1	L	397	ALA	N-CA-C	6.86	114.41	108.78
1	E	359	ASP	O-C-N	-6.86	115.20	123.16
1	I	317	ASP	CA-CB-CG	6.86	119.46	112.60
1	J	379	VAL	N-CA-C	6.85	117.61	110.62
1	B	311	VAL	O-C-N	-6.83	115.69	123.07
1	H	423	ARG	NE-CZ-NH2	6.83	125.35	119.20
1	H	214	ALA	O-C-N	-6.79	114.57	122.93
1	D	212	PRO	CA-C-N	6.78	130.79	120.82
1	D	212	PRO	C-N-CA	6.78	130.79	120.82
1	F	359	ASP	O-C-N	-6.74	115.11	122.79
1	H	426	GLN	O-C-N	-6.73	115.50	122.64
1	B	261	GLU	CA-C-N	6.70	129.25	120.28
1	B	261	GLU	C-N-CA	6.70	129.25	120.28
1	K	171	SER	CA-C-N	6.67	130.06	120.79
1	K	171	SER	C-N-CA	6.67	130.06	120.79
1	J	263	ALA	N-CA-C	6.66	114.24	108.78
1	C	336	ARG	N-CA-CB	6.56	121.57	110.49
1	A	359	ASP	CA-C-N	6.55	133.49	121.70
1	A	359	ASP	C-N-CA	6.55	133.49	121.70
1	H	306	ASP	CA-CB-CG	6.50	119.10	112.60
1	F	304	SER	CA-C-N	6.49	129.51	120.29
1	F	304	SER	C-N-CA	6.49	129.51	120.29
1	G	453	GLY	CA-C-N	6.48	133.37	121.70
1	G	453	GLY	C-N-CA	6.48	133.37	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	230	THR	N-CA-CB	6.48	121.44	110.49
1	L	431	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	F	334	LEU	N-CA-C	6.42	117.97	110.97
1	A	213	ASP	CA-CB-CG	-6.41	106.19	112.60
1	H	359	ASP	O-C-N	-6.40	114.08	122.59
1	L	337	HIS	CA-CB-CG	6.39	120.19	113.80
1	L	257	ASP	CA-CB-CG	6.38	118.98	112.60
1	J	257	ASP	CA-CB-CG	6.38	118.98	112.60
1	L	311	VAL	O-C-N	-6.37	117.23	122.97
1	K	359	ASP	CA-CB-CG	6.36	118.96	112.60
1	C	212	PRO	CA-C-N	6.33	133.63	121.54
1	C	212	PRO	C-N-CA	6.33	133.63	121.54
1	H	336	ARG	O-C-N	-6.33	116.01	123.22
1	E	166	SER	N-CA-C	-6.27	98.19	108.41
1	D	227	THR	CA-C-N	6.25	132.95	121.70
1	D	227	THR	C-N-CA	6.25	132.95	121.70
1	F	431	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	G	364	ASP	N-CA-C	6.23	124.07	110.80
1	I	359	ASP	CA-C-N	6.21	132.88	121.70
1	I	359	ASP	C-N-CA	6.21	132.88	121.70
1	B	232	GLY	CA-C-N	6.21	133.40	121.54
1	B	232	GLY	C-N-CA	6.21	133.40	121.54
1	E	163	GLN	CA-C-N	6.21	132.87	121.70
1	E	163	GLN	C-N-CA	6.21	132.87	121.70
1	H	359	ASP	CA-C-N	6.20	132.86	121.70
1	H	359	ASP	C-N-CA	6.20	132.86	121.70
1	F	374	LYS	O-C-N	-6.20	113.61	121.67
1	F	453	GLY	CA-C-N	6.17	132.81	121.70
1	F	453	GLY	C-N-CA	6.17	132.81	121.70
1	M	426	GLN	CA-C-N	6.17	132.80	121.70
1	M	426	GLN	C-N-CA	6.17	132.80	121.70
1	I	172	GLU	N-CA-C	6.15	118.31	109.14
1	E	374	LYS	O-C-N	-6.14	114.42	122.59
1	E	196	PHE	CA-C-N	6.12	129.40	120.71
1	E	196	PHE	C-N-CA	6.12	129.40	120.71
1	C	408	LYS	CA-C-N	6.11	133.21	121.54
1	C	408	LYS	C-N-CA	6.11	133.21	121.54
1	B	256	THR	CA-C-N	6.08	129.25	120.38
1	B	256	THR	C-N-CA	6.08	129.25	120.38
1	B	453	GLY	CA-C-N	6.06	132.61	121.70
1	B	453	GLY	C-N-CA	6.06	132.61	121.70
1	A	454	THR	CA-CB-OG1	6.06	118.69	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	359	ASP	CA-C-N	6.06	132.60	121.70
1	F	359	ASP	C-N-CA	6.06	132.60	121.70
1	L	332	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	I	374	LYS	O-C-N	-6.03	114.58	122.59
1	L	371	ASP	N-CA-CB	-6.02	101.70	111.22
1	H	184	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	M	453	GLY	N-CA-C	-5.98	104.99	111.21
1	E	359	ASP	CA-C-N	5.96	132.42	121.70
1	E	359	ASP	C-N-CA	5.96	132.42	121.70
1	E	454	THR	CA-C-N	5.95	132.41	121.70
1	E	454	THR	C-N-CA	5.95	132.41	121.70
1	L	351	ASP	N-CA-CB	5.95	118.86	110.12
1	K	336	ARG	N-CA-C	5.93	117.85	110.91
1	D	453	GLY	O-C-N	-5.93	118.96	123.35
1	I	358	GLU	CA-C-N	5.93	132.86	121.54
1	I	358	GLU	C-N-CA	5.93	132.86	121.54
1	C	371	ASP	CB-CA-C	-5.92	101.51	110.92
1	E	424	GLU	CA-C-N	5.91	132.84	121.54
1	E	424	GLU	C-N-CA	5.91	132.84	121.54
1	G	324	ALA	N-CA-C	5.91	118.48	111.33
1	M	426	GLN	O-C-N	-5.90	114.74	122.59
1	B	407	TYR	CA-C-N	5.90	128.67	120.29
1	B	407	TYR	C-N-CA	5.90	128.67	120.29
1	H	453	GLY	CA-C-N	5.89	132.31	121.70
1	H	453	GLY	C-N-CA	5.89	132.31	121.70
1	A	453	GLY	CA-C-N	5.88	132.28	121.70
1	A	453	GLY	C-N-CA	5.88	132.28	121.70
1	A	336	ARG	CA-C-N	5.88	132.28	121.70
1	A	336	ARG	C-N-CA	5.88	132.28	121.70
1	L	213	ASP	CA-CB-CG	5.86	118.46	112.60
1	D	454	THR	CA-C-N	5.86	132.24	121.70
1	D	454	THR	C-N-CA	5.86	132.24	121.70
1	D	359	ASP	O-C-N	-5.85	116.37	123.10
1	A	184	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	D	163	GLN	N-CA-CB	5.83	120.33	110.49
1	M	311	VAL	O-C-N	-5.82	116.44	123.02
1	M	261	GLU	CA-C-N	5.81	128.07	120.28
1	M	261	GLU	C-N-CA	5.81	128.07	120.28
1	G	332	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	G	359	ASP	CA-C-N	5.80	132.13	121.70
1	G	359	ASP	C-N-CA	5.80	132.13	121.70
1	L	274	ARG	NE-CZ-NH2	5.80	124.42	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	THR	N-CA-C	5.79	123.13	110.80
1	L	432	ASP	CA-CB-CG	5.78	118.38	112.60
1	I	324	ALA	CA-C-N	5.77	128.01	120.28
1	I	324	ALA	C-N-CA	5.77	128.01	120.28
1	J	408	LYS	CA-C-N	5.75	129.06	120.31
1	J	408	LYS	C-N-CA	5.75	129.06	120.31
1	L	323	THR	N-CA-CB	5.75	118.49	110.04
1	G	454	THR	CA-C-N	5.74	132.03	121.70
1	G	454	THR	C-N-CA	5.74	132.03	121.70
1	K	317	ASP	CA-CB-CG	-5.74	106.86	112.60
1	K	385	LEU	N-CA-C	5.72	117.79	109.84
1	I	334	LEU	N-CA-C	5.71	117.18	111.07
1	D	308	ALA	N-CA-C	5.70	117.49	111.28
1	D	309	LYS	N-CA-C	5.69	117.89	110.43
1	D	256	THR	CA-C-N	5.69	127.83	120.44
1	D	256	THR	C-N-CA	5.69	127.83	120.44
1	K	336	ARG	CA-C-N	5.67	131.91	121.70
1	K	336	ARG	C-N-CA	5.67	131.91	121.70
1	K	359	ASP	CA-C-N	5.67	131.90	121.70
1	K	359	ASP	C-N-CA	5.67	131.90	121.70
1	E	301	THR	CA-C-N	5.67	127.87	120.28
1	E	301	THR	C-N-CA	5.67	127.87	120.28
1	E	326	THR	CA-C-N	5.67	128.22	120.46
1	E	326	THR	C-N-CA	5.67	128.22	120.46
1	E	335	GLY	CA-C-N	5.66	128.75	120.71
1	E	335	GLY	C-N-CA	5.66	128.75	120.71
1	E	229	THR	CA-C-N	5.65	132.33	121.54
1	E	229	THR	C-N-CA	5.65	132.33	121.54
1	K	304	SER	CA-C-N	5.65	128.12	120.44
1	K	304	SER	C-N-CA	5.65	128.12	120.44
1	M	372	SER	O-C-N	-5.64	116.15	123.32
1	L	409	ASP	CA-CB-CG	5.62	118.22	112.60
1	M	240	LYS	N-CA-C	5.61	117.40	111.28
1	G	306	ASP	CA-C-N	5.59	132.22	121.54
1	G	306	ASP	C-N-CA	5.59	132.22	121.54
1	I	453	GLY	CA-C-N	5.58	131.75	121.70
1	I	453	GLY	C-N-CA	5.58	131.75	121.70
1	D	171	SER	CA-C-N	5.58	132.19	121.54
1	D	171	SER	C-N-CA	5.58	132.19	121.54
1	F	363	GLN	CA-C-N	5.57	132.19	121.54
1	F	363	GLN	C-N-CA	5.57	132.19	121.54
1	J	184	ARG	CA-C-N	5.57	130.29	120.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	184	ARG	C-N-CA	5.57	130.29	120.87
1	G	332	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	L	363	GLN	CA-C-N	5.57	132.17	121.54
1	L	363	GLN	C-N-CA	5.57	132.17	121.54
1	M	227	THR	CA-C-N	5.56	131.71	121.70
1	M	227	THR	C-N-CA	5.56	131.71	121.70
1	G	204	LYS	N-CA-C	5.56	117.02	111.07
1	L	163	GLN	O-C-N	-5.56	116.88	123.22
1	C	214	ALA	N-CA-C	5.56	117.80	108.96
1	G	326	THR	CA-C-N	5.54	128.06	120.46
1	G	326	THR	C-N-CA	5.54	128.06	120.46
1	E	359	ASP	CA-CB-CG	5.54	118.14	112.60
1	G	276	ILE	CA-C-N	5.54	127.70	120.28
1	G	276	ILE	C-N-CA	5.54	127.70	120.28
1	G	214	ALA	O-C-N	-5.53	116.94	123.41
1	M	367	GLN	O-C-N	-5.52	116.88	123.06
1	B	185	ASP	N-CA-C	5.52	117.29	111.28
1	H	454	THR	CA-C-N	5.51	131.61	121.70
1	H	454	THR	C-N-CA	5.51	131.61	121.70
1	K	358	GLU	CA-C-N	5.51	128.53	120.71
1	K	358	GLU	C-N-CA	5.51	128.53	120.71
1	B	452	SER	CA-C-O	5.50	121.13	117.94
1	C	227	THR	CA-C-N	5.48	131.57	121.70
1	C	227	THR	C-N-CA	5.48	131.57	121.70
1	H	244	PHE	CA-CB-CG	-5.48	108.32	113.80
1	K	172	GLU	N-CA-C	5.48	117.71	111.02
1	D	191	VAL	N-CA-C	5.48	116.21	110.62
1	A	324	ALA	N-CA-C	5.47	118.75	111.75
1	M	372	SER	N-CA-C	5.47	117.86	111.02
1	L	223	SER	N-CA-C	5.46	117.23	111.28
1	A	359	ASP	O-C-N	-5.46	115.33	122.59
1	F	172	GLU	O-C-N	-5.44	117.31	123.13
1	K	426	GLN	O-C-N	-5.44	116.75	123.44
1	B	214	ALA	O-C-N	-5.44	116.12	122.81
1	M	351	ASP	N-CA-CB	-5.44	101.84	109.94
1	B	227	THR	CA-C-N	5.43	131.48	121.70
1	B	227	THR	C-N-CA	5.43	131.48	121.70
1	K	378	GLN	N-CA-C	5.43	118.73	111.24
1	I	360	GLU	CB-CA-C	5.41	120.38	110.10
1	C	261	GLU	CA-C-N	5.41	127.53	120.28
1	C	261	GLU	C-N-CA	5.41	127.53	120.28
1	F	454	THR	CA-C-N	5.41	131.44	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	454	THR	C-N-CA	5.41	131.44	121.70
1	L	374	LYS	CA-C-N	5.41	131.43	121.70
1	L	374	LYS	C-N-CA	5.41	131.43	121.70
1	M	444	ARG	NE-CZ-NH2	5.41	124.06	119.20
1	K	453	GLY	CA-C-N	5.40	131.42	121.70
1	K	453	GLY	C-N-CA	5.40	131.42	121.70
1	B	166	SER	O-C-N	-5.40	115.99	123.01
1	J	374	LYS	CA-C-N	5.40	131.41	121.70
1	J	374	LYS	C-N-CA	5.40	131.41	121.70
1	I	332	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	D	290	GLY	CA-C-N	5.38	127.92	120.29
1	D	290	GLY	C-N-CA	5.38	127.92	120.29
1	M	350	MET	CA-C-N	5.36	127.78	120.54
1	M	350	MET	C-N-CA	5.36	127.78	120.54
1	L	454	THR	CA-C-N	5.36	131.34	121.70
1	L	454	THR	C-N-CA	5.36	131.34	121.70
1	B	429	LYS	N-CA-C	5.34	122.18	110.80
1	H	374	LYS	O-C-N	-5.34	114.95	122.10
1	E	336	ARG	O-C-N	-5.33	116.31	122.87
1	C	325	LYS	N-CA-C	5.33	119.27	112.34
1	E	355	ASP	CA-CB-CG	-5.33	107.27	112.60
1	J	268	LEU	O-C-N	-5.33	115.19	121.32
1	F	351	ASP	CA-C-N	5.33	127.95	120.28
1	F	351	ASP	C-N-CA	5.33	127.95	120.28
1	L	334	LEU	N-CA-C	5.33	116.77	111.07
1	F	439	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	I	227	THR	CA-C-N	5.32	131.28	121.70
1	I	227	THR	C-N-CA	5.32	131.28	121.70
1	A	256	THR	CA-C-N	5.32	127.41	120.28
1	A	256	THR	C-N-CA	5.32	127.41	120.28
1	B	336	ARG	CA-C-N	5.32	131.27	121.70
1	B	336	ARG	C-N-CA	5.32	131.27	121.70
1	F	188	LYS	CA-C-N	5.32	127.35	120.44
1	F	188	LYS	C-N-CA	5.32	127.35	120.44
1	B	235	VAL	CA-C-N	5.31	131.69	121.54
1	B	235	VAL	C-N-CA	5.31	131.69	121.54
1	E	228	ASP	CB-CA-C	5.30	120.17	110.10
1	C	362	TRP	CG-CD2-CE3	-5.30	128.60	133.90
1	G	359	ASP	CA-CB-CG	5.30	117.90	112.60
1	H	304	SER	CA-C-N	5.29	127.64	120.44
1	H	304	SER	C-N-CA	5.29	127.64	120.44
1	M	184	ARG	NE-CZ-NH2	5.29	123.96	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	261	GLU	CA-C-N	5.29	127.80	120.29
1	J	261	GLU	C-N-CA	5.29	127.80	120.29
1	C	309	LYS	N-CA-C	5.27	117.34	110.43
1	L	304	SER	CA-C-N	5.27	127.34	120.28
1	L	304	SER	C-N-CA	5.27	127.34	120.28
1	K	222	ALA	CA-C-N	5.27	127.34	120.28
1	K	222	ALA	C-N-CA	5.27	127.34	120.28
1	B	233	GLU	N-CA-CB	5.26	119.39	110.49
1	C	224	THR	N-CA-C	5.26	116.72	110.19
1	E	176	THR	N-CA-C	5.26	117.86	110.23
1	L	227	THR	CA-C-N	5.25	131.15	121.70
1	L	227	THR	C-N-CA	5.25	131.15	121.70
1	J	364	ASP	N-CA-C	5.24	121.97	110.80
1	M	218	THR	N-CA-CB	5.24	117.66	109.85
1	D	306	ASP	CA-C-N	5.24	131.54	121.54
1	D	306	ASP	C-N-CA	5.24	131.54	121.54
1	M	395	ALA	CA-C-N	5.24	131.54	121.54
1	M	395	ALA	C-N-CA	5.24	131.54	121.54
1	B	430	GLN	CA-C-N	5.23	131.54	121.54
1	B	430	GLN	C-N-CA	5.23	131.54	121.54
1	M	165	SER	CA-C-N	5.22	131.10	121.70
1	M	165	SER	C-N-CA	5.22	131.10	121.70
1	M	240	LYS	CA-C-N	5.22	131.10	121.70
1	M	240	LYS	C-N-CA	5.22	131.10	121.70
1	F	214	ALA	O-C-N	-5.22	117.13	123.29
1	G	268	LEU	O-C-N	-5.22	115.81	120.71
1	B	324	ALA	N-CA-C	5.21	119.12	112.87
1	M	299	LEU	N-CA-C	5.21	116.96	111.28
1	B	227	THR	O-C-N	-5.19	116.73	122.91
1	J	311	VAL	O-C-N	-5.19	117.99	123.03
1	I	411	PHE	N-CA-CB	5.19	119.27	110.49
1	K	396	LYS	N-CA-C	5.19	121.86	110.80
1	A	173	SER	CA-C-N	5.17	131.41	121.54
1	A	173	SER	C-N-CA	5.17	131.41	121.54
1	I	374	LYS	CA-C-N	5.17	131.41	121.54
1	I	374	LYS	C-N-CA	5.17	131.41	121.54
1	C	431	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	H	263	ALA	N-CA-C	5.16	113.70	108.75
1	A	311	VAL	CA-C-N	5.16	130.98	121.70
1	A	311	VAL	C-N-CA	5.16	130.98	121.70
1	F	413	MET	CA-C-N	5.16	125.45	119.93
1	F	413	MET	C-N-CA	5.16	125.45	119.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	439	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	I	431	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	G	232	GLY	CA-C-N	5.14	131.36	121.54
1	G	232	GLY	C-N-CA	5.14	131.36	121.54
1	C	426	GLN	O-C-N	-5.14	117.30	123.31
1	I	291	ASP	N-CA-CB	-5.14	101.81	110.49
1	I	306	ASP	CA-C-N	5.13	131.34	121.54
1	I	306	ASP	C-N-CA	5.13	131.34	121.54
1	E	311	VAL	O-C-N	-5.13	117.53	123.07
1	M	307	SER	N-CA-CB	5.12	119.14	110.49
1	K	316	ALA	CA-C-N	5.11	131.31	121.54
1	K	316	ALA	C-N-CA	5.11	131.31	121.54
1	M	235	VAL	N-CA-C	5.10	119.96	109.34
1	G	274	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	350	MET	CA-C-N	5.10	127.37	120.44
1	A	350	MET	C-N-CA	5.10	127.37	120.44
1	F	290	GLY	CA-C-N	5.09	127.37	120.44
1	F	290	GLY	C-N-CA	5.09	127.37	120.44
1	E	445	TYR	N-CA-C	5.09	116.64	111.14
1	A	454	THR	CA-C-N	5.09	130.86	121.70
1	A	454	THR	C-N-CA	5.09	130.86	121.70
1	H	332	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	H	184	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	K	360	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	311	VAL	O-C-N	-5.08	117.59	123.07
1	J	426	GLN	CA-C-N	5.07	130.83	121.70
1	J	426	GLN	C-N-CA	5.07	130.83	121.70
1	B	257	ASP	CA-CB-CG	5.07	117.67	112.60
1	G	360	GLU	CA-C-N	5.07	131.21	121.54
1	G	360	GLU	C-N-CA	5.07	131.21	121.54
1	K	243	HIS	CA-CB-CG	5.06	118.86	113.80
1	C	453	GLY	CA-C-N	5.05	130.80	121.70
1	C	453	GLY	C-N-CA	5.05	130.80	121.70
1	K	359	ASP	O-C-N	-5.05	116.66	122.87
1	K	339	LEU	CA-C-N	5.05	129.58	122.46
1	K	339	LEU	C-N-CA	5.05	129.58	122.46
1	J	370	ASN	CA-CB-CG	5.05	117.65	112.60
1	G	299	LEU	N-CA-C	5.04	116.86	111.36
1	B	222	ALA	CA-C-N	5.04	127.45	120.29
1	B	222	ALA	C-N-CA	5.04	127.45	120.29
1	L	412	VAL	N-CA-C	5.04	119.83	109.34
1	K	411	PHE	CA-CB-CG	-5.04	108.76	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	E	336	ARG	CA-C-N	5.03	130.75	121.70
1	E	336	ARG	C-N-CA	5.03	130.75	121.70
1	C	227	THR	O-C-N	-5.02	116.32	122.55
1	A	336	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	K	274	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	M	361	GLU	CA-C-N	5.01	130.72	121.70
1	M	361	GLU	C-N-CA	5.01	130.72	121.70
1	E	163	GLN	O-C-N	-5.01	117.46	123.27
1	H	349	SER	N-CA-C	5.01	116.99	110.43
1	D	307	SER	N-CA-CB	5.01	118.95	110.49

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ARG	Sidechain
1	A	184	ARG	Sidechain
1	A	187	GLN	Peptide
1	A	370	ASN	Peptide
1	A	374	LYS	Peptide
1	A	381	ARG	Sidechain
1	A	409	ASP	Peptide
1	A	417	ARG	Sidechain
1	A	423	ARG	Sidechain
1	A	434	TYR	Sidechain
1	B	184	ARG	Sidechain
1	B	336	ARG	Sidechain
1	B	381	ARG	Sidechain
1	B	407	TYR	Sidechain
1	B	434	TYR	Sidechain
1	B	444	ARG	Sidechain
1	C	229	THR	Peptide
1	C	232	GLY	Peptide
1	C	274	ARG	Sidechain
1	C	331	ARG	Sidechain
1	C	332	ARG	Sidechain
1	C	338	GLY	Peptide
1	C	353	TYR	Sidechain
1	C	415	ARG	Sidechain
1	C	417	ARG	Sidechain
1	C	425	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	434	TYR	Sidechain
1	C	444	ARG	Sidechain
1	D	184	ARG	Sidechain
1	D	227	THR	Peptide
1	D	332	ARG	Sidechain
1	D	417	ARG	Sidechain
1	D	434	TYR	Sidechain
1	D	455	TYR	Sidechain
1	E	165	SER	Peptide
1	E	184	ARG	Sidechain
1	E	332	ARG	Sidechain
1	E	392	TYR	Sidechain
1	E	407	TYR	Sidechain
1	E	423	ARG	Sidechain
1	E	425	ARG	Sidechain
1	E	434	TYR	Sidechain
1	E	455	TYR	Sidechain
1	F	172	GLU	Peptide
1	F	184	ARG	Sidechain
1	F	212	PRO	Peptide
1	F	274	ARG	Sidechain
1	F	415	ARG	Sidechain
1	F	417	ARG	Sidechain
1	F	423	ARG	Sidechain
1	F	431	ARG	Sidechain
1	F	439	ARG	Sidechain
1	G	160	ALA	Peptide
1	G	184	ARG	Sidechain
1	G	332	ARG	Sidechain
1	G	358	GLU	Peptide
1	G	431	ARG	Peptide
1	G	455	TYR	Sidechain
1	H	181	ARG	Sidechain
1	H	332	ARG	Sidechain
1	H	423	ARG	Sidechain
1	H	425	ARG	Sidechain
1	H	431	ARG	Sidechain
1	I	181	ARG	Sidechain
1	I	184	ARG	Sidechain
1	I	290	GLY	Peptide
1	I	332	ARG	Sidechain
1	I	374	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	I	392	TYR	Sidechain
1	I	409	ASP	Peptide
1	I	417	ARG	Sidechain
1	I	434	TYR	Sidechain
1	J	274	ARG	Sidechain
1	J	332	ARG	Sidechain
1	J	354	TYR	Sidechain
1	J	407	TYR	Sidechain
1	J	444	ARG	Sidechain
1	K	213	ASP	Peptide
1	K	358	GLU	Peptide
1	K	417	ARG	Sidechain
1	K	431	ARG	Peptide
1	K	445	TYR	Sidechain
1	L	274	ARG	Sidechain
1	L	332	ARG	Sidechain
1	L	354	TYR	Sidechain
1	L	392	TYR	Sidechain
1	L	431	ARG	Sidechain
1	L	434	TYR	Sidechain
1	M	331	ARG	Sidechain
1	M	417	ARG	Sidechain
1	M	425	ARG	Sidechain
1	M	439	ARG	Sidechain
1	M	444	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2317	2345	2342	0	0
1	B	2317	2345	2342	0	0
1	C	2317	2345	2342	0	0
1	D	2317	2345	2342	0	0
1	E	2317	2345	2342	0	0
1	F	2317	2345	2342	0	0
1	G	2317	2345	2342	0	0
1	H	2317	2345	2342	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2317	2345	2342	0	0
1	J	2317	2345	2342	0	0
1	K	2317	2345	2342	0	0
1	L	2317	2345	2342	0	0
1	M	2288	2315	2314	0	0
All	All	30092	30455	30418	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/299 (99%)	233 (78%)	42 (14%)	22 (7%)	1	11
1	B	297/299 (99%)	233 (78%)	47 (16%)	17 (6%)	1	15
1	C	297/299 (99%)	231 (78%)	45 (15%)	21 (7%)	1	12
1	D	297/299 (99%)	232 (78%)	46 (16%)	19 (6%)	1	14
1	E	297/299 (99%)	221 (74%)	54 (18%)	22 (7%)	1	11
1	F	297/299 (99%)	227 (76%)	43 (14%)	27 (9%)	0	8
1	G	297/299 (99%)	237 (80%)	43 (14%)	17 (6%)	1	15
1	H	297/299 (99%)	226 (76%)	54 (18%)	17 (6%)	1	15
1	I	297/299 (99%)	226 (76%)	48 (16%)	23 (8%)	1	11
1	J	297/299 (99%)	234 (79%)	48 (16%)	15 (5%)	1	17
1	K	297/299 (99%)	229 (77%)	47 (16%)	21 (7%)	1	12
1	L	297/299 (99%)	235 (79%)	46 (16%)	16 (5%)	1	16
1	M	293/299 (98%)	222 (76%)	42 (14%)	29 (10%)	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3857/3887 (99%)	2986 (77%)	605 (16%)	266 (7%)	2	12

All (266) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	A	174	TYR
1	A	230	THR
1	A	309	LYS
1	A	364	ASP
1	A	431	ARG
1	B	213	ASP
1	B	233	GLU
1	B	236	LYS
1	B	333	LYS
1	B	340	LYS
1	C	216	LYS
1	C	336	ARG
1	C	372	SER
1	C	409	ASP
1	D	172	GLU
1	D	228	ASP
1	D	307	SER
1	D	372	SER
1	E	408	LYS
1	E	429	LYS
1	F	213	ASP
1	F	235	VAL
1	F	307	SER
1	F	311	VAL
1	F	315	LYS
1	G	162	ASN
1	G	174	TYR
1	G	307	SER
1	G	361	GLU
1	G	362	TRP
1	G	364	ASP
1	H	266	SER
1	H	397	ALA
1	I	319	SER
1	I	372	SER
1	I	375	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	268	LEU
1	J	364	ASP
1	K	317	ASP
1	K	323	THR
1	K	361	GLU
1	L	364	ASP
1	L	408	LYS
1	M	171	SER
1	M	366	ALA
1	M	396	LYS
1	M	397	ALA
1	M	431	ARG
1	A	175	GLU
1	A	231	THR
1	A	264	ILE
1	A	323	THR
1	A	361	GLU
1	B	260	GLU
1	B	360	GLU
1	B	372	SER
1	B	397	ALA
1	B	406	VAL
1	B	411	PHE
1	C	231	THR
1	C	233	GLU
1	C	236	LYS
1	C	308	ALA
1	C	343	LYS
1	C	356	LEU
1	C	364	ASP
1	C	378	GLN
1	D	174	TYR
1	D	185	ASP
1	D	188	LYS
1	D	364	ASP
1	D	425	ARG
1	E	164	SER
1	E	230	THR
1	E	335	GLY
1	E	362	TRP
1	E	364	ASP
1	E	396	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	412	VAL
1	E	425	ARG
1	F	186	LEU
1	F	190	LEU
1	F	203	SER
1	F	220	VAL
1	F	340	LYS
1	F	367	GLN
1	F	378	GLN
1	F	394	PRO
1	F	409	ASP
1	G	213	ASP
1	G	304	SER
1	G	317	ASP
1	G	450	VAL
1	G	455	TYR
1	H	361	GLU
1	H	364	ASP
1	I	307	SER
1	I	308	ALA
1	I	364	ASP
1	I	412	VAL
1	I	425	ARG
1	I	457	ALA
1	J	213	ASP
1	J	321	LEU
1	J	371	ASP
1	K	257	ASP
1	K	315	LYS
1	K	411	PHE
1	L	313	GLU
1	L	336	ARG
1	L	356	LEU
1	L	411	PHE
1	L	412	VAL
1	M	173	SER
1	M	225	TYR
1	M	235	VAL
1	M	264	ILE
1	M	317	ASP
1	M	324	ALA
1	M	334	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	379	VAL
1	M	411	PHE
1	A	162	ASN
1	A	263	ALA
1	A	371	ASP
1	A	382	ILE
1	A	397	ALA
1	B	407	TYR
1	C	215	GLY
1	C	232	GLY
1	C	398	ASN
1	C	457	ALA
1	D	233	GLU
1	D	258	GLU
1	D	336	ARG
1	D	430	GLN
1	E	172	GLU
1	E	174	TYR
1	E	204	LYS
1	E	222	ALA
1	E	232	GLY
1	E	319	SER
1	E	340	LYS
1	E	361	GLU
1	E	411	PHE
1	F	227	THR
1	F	319	SER
1	F	336	ARG
1	F	339	LEU
1	F	364	ASP
1	G	215	GLY
1	G	397	ALA
1	H	175	GLU
1	H	233	GLU
1	H	317	ASP
1	H	340	LYS
1	H	371	ASP
1	I	292	GLY
1	I	359	ASP
1	I	374	LYS
1	I	377	GLY
1	I	411	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	341	LEU
1	J	357	LEU
1	J	425	ARG
1	J	445	TYR
1	K	188	LYS
1	K	212	PRO
1	K	258	GLU
1	K	356	LEU
1	K	364	ASP
1	K	394	PRO
1	K	396	LYS
1	K	397	ALA
1	K	425	ARG
1	K	454	THR
1	L	318	GLY
1	L	352	ALA
1	L	400	ALA
1	L	428	GLY
1	M	185	ASP
1	M	360	GLU
1	M	374	LYS
1	A	168	GLU
1	A	186	LEU
1	A	430	GLN
1	B	228	ASP
1	B	395	ALA
1	C	408	LYS
1	C	449	GLY
1	D	162	ASN
1	D	229	THR
1	D	371	ASP
1	E	324	ALA
1	F	341	LEU
1	F	342	SER
1	F	372	SER
1	F	411	PHE
1	F	445	TYR
1	F	455	TYR
1	G	343	LYS
1	G	418	ALA
1	H	168	GLU
1	H	222	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	359	ASP
1	H	411	PHE
1	I	212	PRO
1	I	318	GLY
1	I	430	GLN
1	J	316	ALA
1	K	260	GLU
1	K	446	PHE
1	L	212	PRO
1	L	317	ASP
1	L	399	SER
1	M	166	SER
1	M	216	LYS
1	M	304	SER
1	M	429	LYS
1	M	449	GLY
1	M	455	TYR
1	A	213	ASP
1	B	174	TYR
1	B	431	ARG
1	C	425	ARG
1	D	317	ASP
1	D	341	LEU
1	F	430	GLN
1	G	457	ALA
1	H	316	ALA
1	H	409	ASP
1	I	174	TYR
1	I	187	GLN
1	I	203	SER
1	I	214	ALA
1	I	397	ALA
1	J	187	GLN
1	J	317	ASP
1	J	362	TRP
1	K	379	VAL
1	K	448	ASN
1	L	410	ASN
1	M	188	LYS
1	M	214	ALA
1	M	376	GLN
1	M	399	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	185	ASP
1	B	161	VAL
1	C	213	ASP
1	D	316	ALA
1	G	430	GLN
1	H	171	SER
1	K	170	SER
1	M	165	SER
1	F	191	VAL
1	H	212	PRO
1	L	191	VAL
1	C	338	GLY
1	E	215	GLY
1	I	193	GLY
1	J	335	GLY
1	J	212	PRO
1	A	373	VAL
1	E	373	VAL
1	M	212	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	250/250 (100%)	239 (96%)	11 (4%)	25	49	
1	B	250/250 (100%)	235 (94%)	15 (6%)	17	43	
1	C	250/250 (100%)	232 (93%)	18 (7%)	13	39	
1	D	250/250 (100%)	237 (95%)	13 (5%)	21	46	
1	E	250/250 (100%)	238 (95%)	12 (5%)	23	47	
1	F	250/250 (100%)	236 (94%)	14 (6%)	19	45	
1	G	250/250 (100%)	237 (95%)	13 (5%)	21	46	
1	H	250/250 (100%)	230 (92%)	20 (8%)	11	36	
1	I	250/250 (100%)	237 (95%)	13 (5%)	21	46	

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	250/250 (100%)	231 (92%)	19 (8%)	12	37
1	K	250/250 (100%)	238 (95%)	12 (5%)	23	47
1	L	250/250 (100%)	234 (94%)	16 (6%)	16	42
1	M	247/250 (99%)	233 (94%)	14 (6%)	18	44
All	All	3247/3250 (100%)	3057 (94%)	190 (6%)	19	43

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	165	SER
1	A	258	GLU
1	A	260	GLU
1	A	277	GLU
1	A	291	ASP
1	A	336	ARG
1	A	339	LEU
1	A	370	ASN
1	A	430	GLN
1	A	454	THR
1	B	179	SER
1	B	186	LEU
1	B	189	GLU
1	B	213	ASP
1	B	233	GLU
1	B	257	ASP
1	B	313	GLU
1	B	361	GLU
1	B	374	LYS
1	B	406	VAL
1	B	408	LYS
1	B	409	ASP
1	B	425	ARG
1	B	432	ASP
1	B	454	THR
1	C	175	GLU
1	C	256	THR
1	C	257	ASP
1	C	260	GLU
1	C	291	ASP
1	C	306	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	310	VAL
1	C	313	GLU
1	C	323	THR
1	C	340	LYS
1	C	360	GLU
1	C	391	GLU
1	C	396	LYS
1	C	408	LYS
1	C	409	ASP
1	C	437	THR
1	C	443	GLN
1	C	450	VAL
1	D	163	GLN
1	D	187	GLN
1	D	234	GLU
1	D	257	ASP
1	D	277	GLU
1	D	301	THR
1	D	306	ASP
1	D	315	LYS
1	D	332	ARG
1	D	355	ASP
1	D	356	LEU
1	D	359	ASP
1	D	454	THR
1	E	165	SER
1	E	175	GLU
1	E	228	ASP
1	E	233	GLU
1	E	249	LEU
1	E	291	ASP
1	E	306	ASP
1	E	317	ASP
1	E	375	LEU
1	E	406	VAL
1	E	422	GLU
1	E	424	GLU
1	F	163	GLN
1	F	172	GLU
1	F	173	SER
1	F	176	THR
1	F	213	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	234	GLU
1	F	261	GLU
1	F	279	HIS
1	F	291	ASP
1	F	351	ASP
1	F	360	GLU
1	F	363	GLN
1	F	367	GLN
1	F	409	ASP
1	G	172	GLU
1	G	175	GLU
1	G	210	VAL
1	G	260	GLU
1	G	279	HIS
1	G	325	LYS
1	G	355	ASP
1	G	358	GLU
1	G	360	GLU
1	G	363	GLN
1	G	391	GLU
1	G	408	LYS
1	G	409	ASP
1	H	172	GLU
1	H	175	GLU
1	H	183	ILE
1	H	186	LEU
1	H	187	GLN
1	H	234	GLU
1	H	289	THR
1	H	306	ASP
1	H	315	LYS
1	H	343	LYS
1	H	351	ASP
1	H	357	LEU
1	H	364	ASP
1	H	391	GLU
1	H	404	VAL
1	H	412	VAL
1	H	422	GLU
1	H	432	ASP
1	H	437	THR
1	H	454	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	213	ASP
1	I	285	GLU
1	I	309	LYS
1	I	317	ASP
1	I	319	SER
1	I	323	THR
1	I	350	MET
1	I	355	ASP
1	I	360	GLU
1	I	363	GLN
1	I	401	GLU
1	I	406	VAL
1	I	408	LYS
1	J	175	GLU
1	J	185	ASP
1	J	189	GLU
1	J	228	ASP
1	J	234	GLU
1	J	257	ASP
1	J	291	ASP
1	J	330	LEU
1	J	358	GLU
1	J	360	GLU
1	J	362	TRP
1	J	368	VAL
1	J	370	ASN
1	J	374	LYS
1	J	378	GLN
1	J	382	ILE
1	J	422	GLU
1	J	424	GLU
1	J	437	THR
1	K	172	GLU
1	K	175	GLU
1	K	241	GLU
1	K	301	THR
1	K	311	VAL
1	K	313	GLU
1	K	315	LYS
1	K	351	ASP
1	K	359	ASP
1	K	360	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	363	GLN
1	K	451	VAL
1	L	172	GLU
1	L	175	GLU
1	L	185	ASP
1	L	233	GLU
1	L	258	GLU
1	L	304	SER
1	L	305	GLU
1	L	310	VAL
1	L	323	THR
1	L	342	SER
1	L	359	ASP
1	L	396	LYS
1	L	408	LYS
1	L	421	VAL
1	L	424	GLU
1	L	440	VAL
1	M	172	GLU
1	M	173	SER
1	M	205	ILE
1	M	257	ASP
1	M	258	GLU
1	M	304	SER
1	M	313	GLU
1	M	374	LYS
1	M	379	VAL
1	M	398	ASN
1	M	401	GLU
1	M	406	VAL
1	M	432	ASP
1	M	454	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

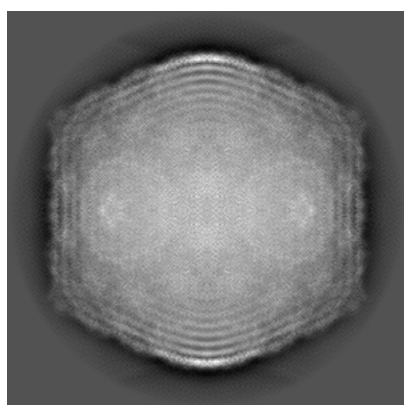
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20125. These allow visual inspection of the internal detail of the map and identification of artifacts.

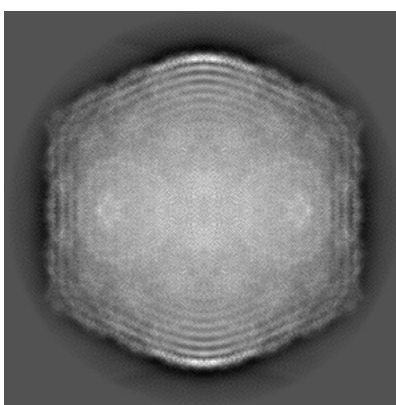
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

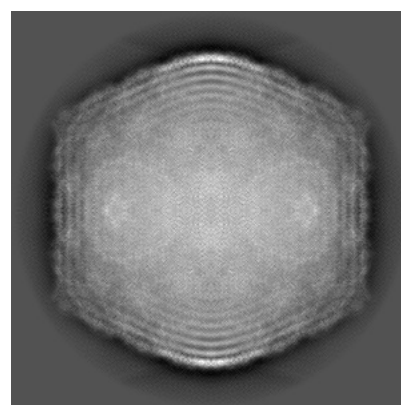
6.1.1 Primary map



X



Y

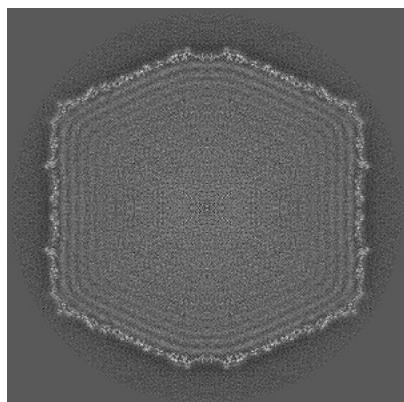


Z

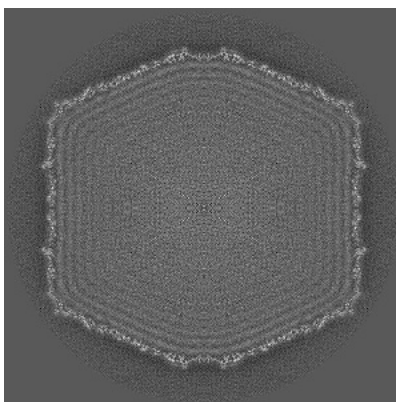
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

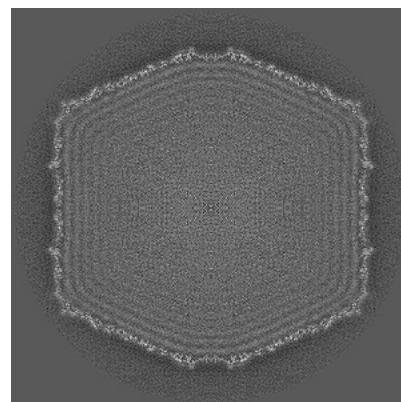
6.2.1 Primary map



X Index: 375



Y Index: 375

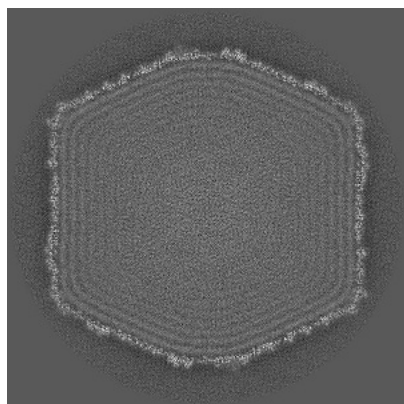


Z Index: 375

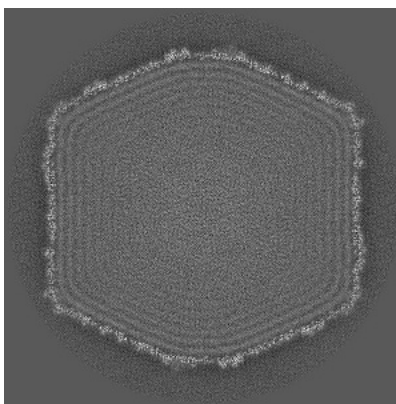
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

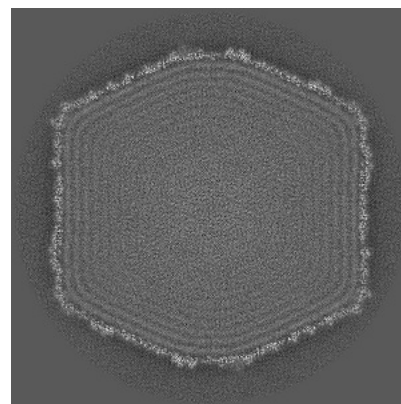
6.3.1 Primary map



X Index: 382



Y Index: 368

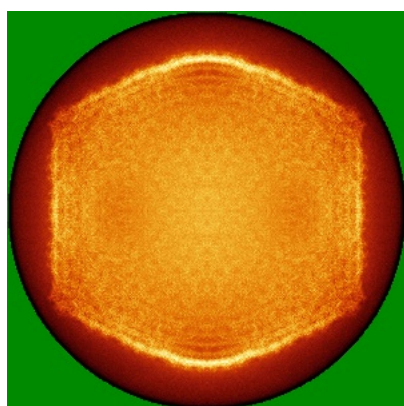


Z Index: 382

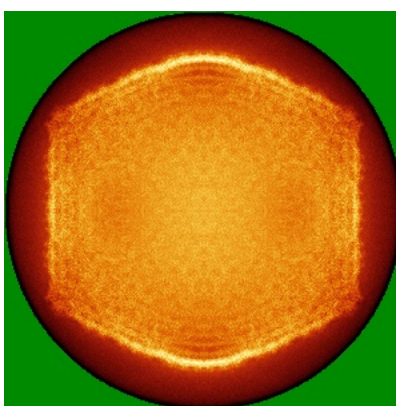
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

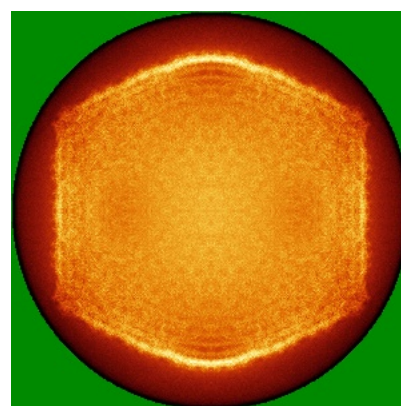
6.4.1 Primary map



X



Y

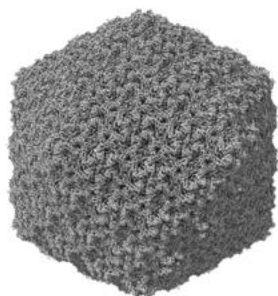


Z

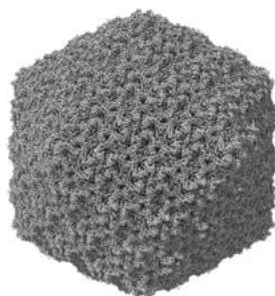
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

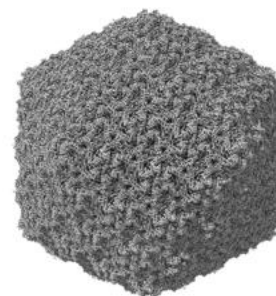
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

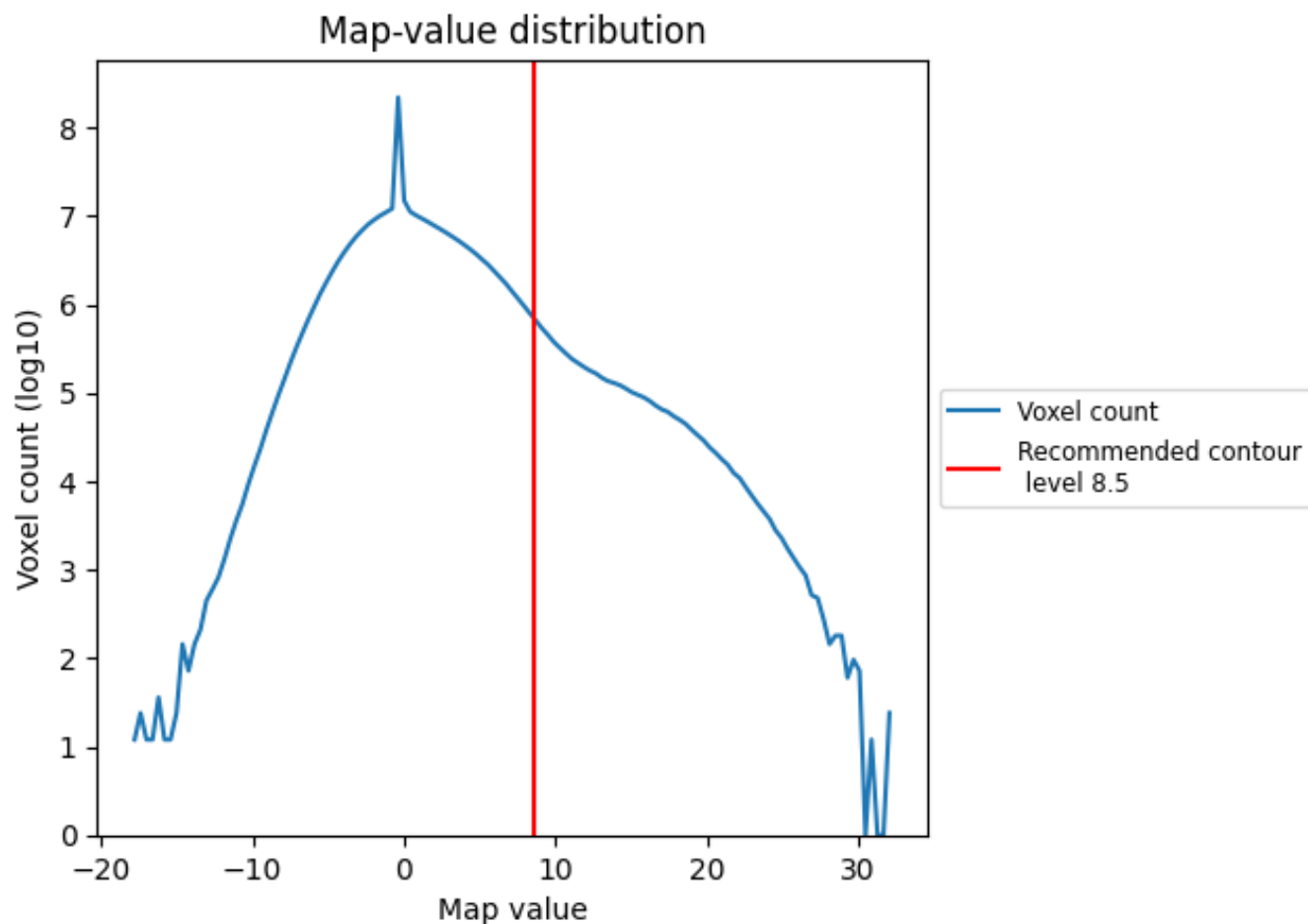
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

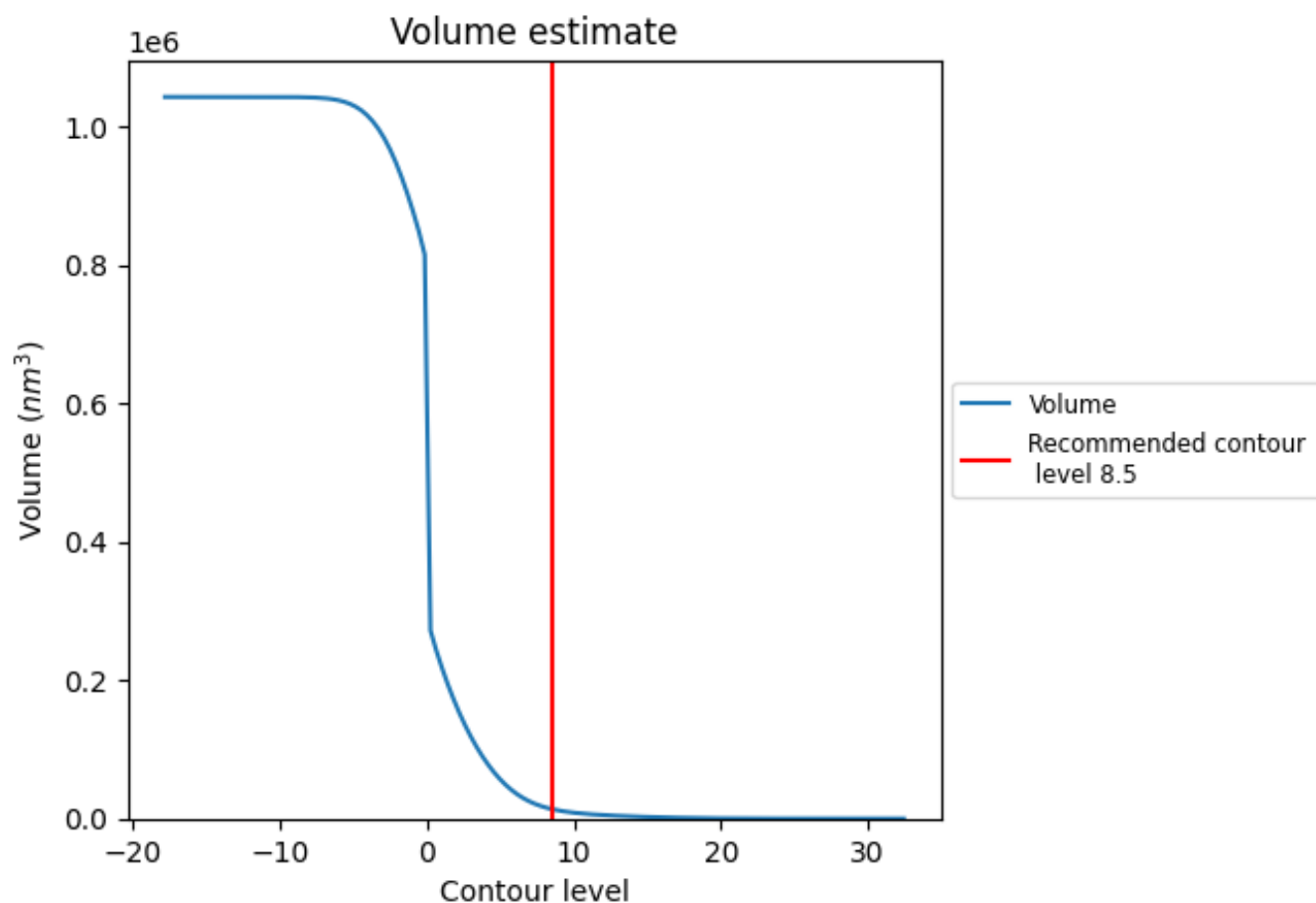
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

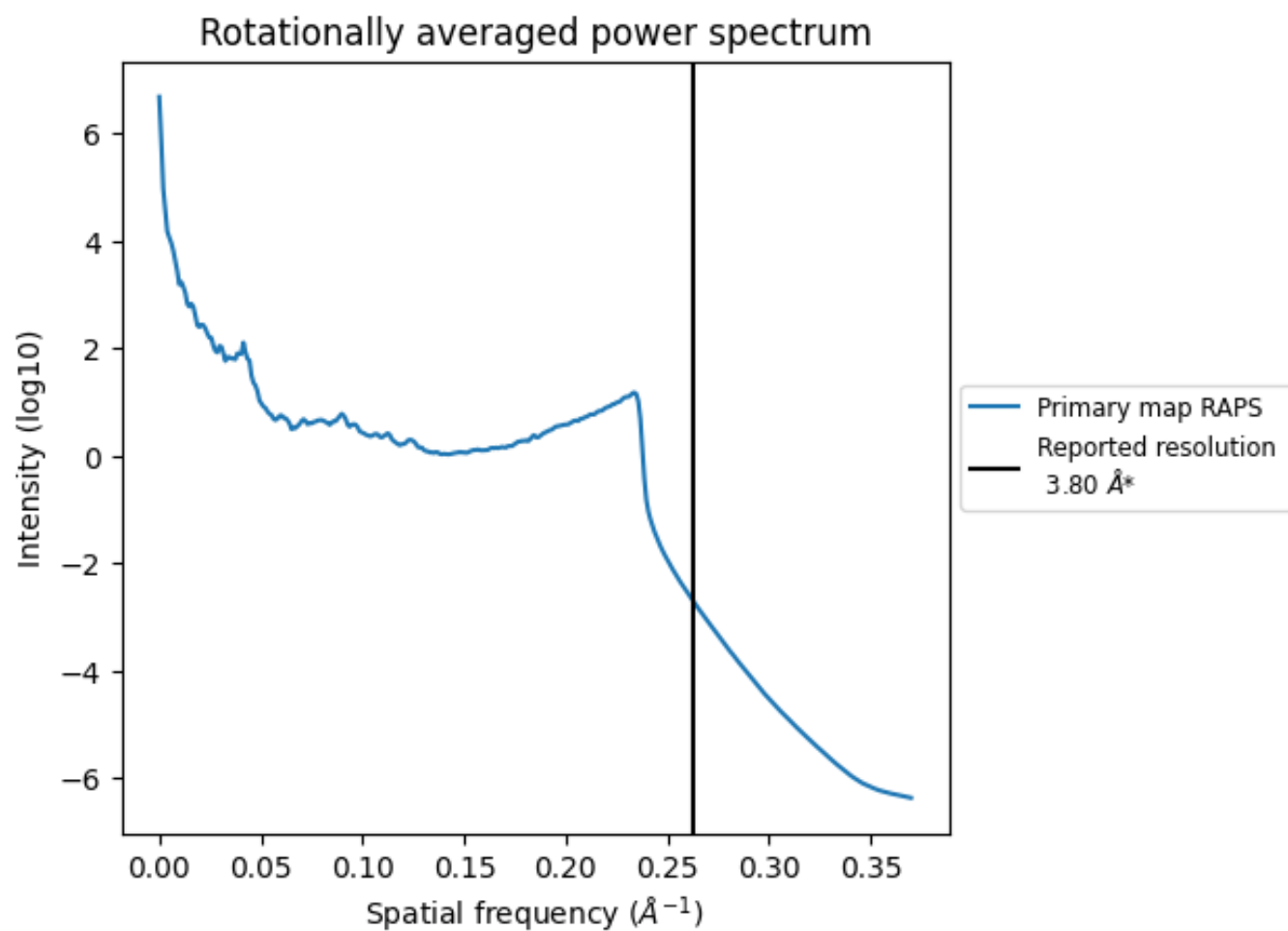
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13798 nm³; this corresponds to an approximate mass of 12464 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

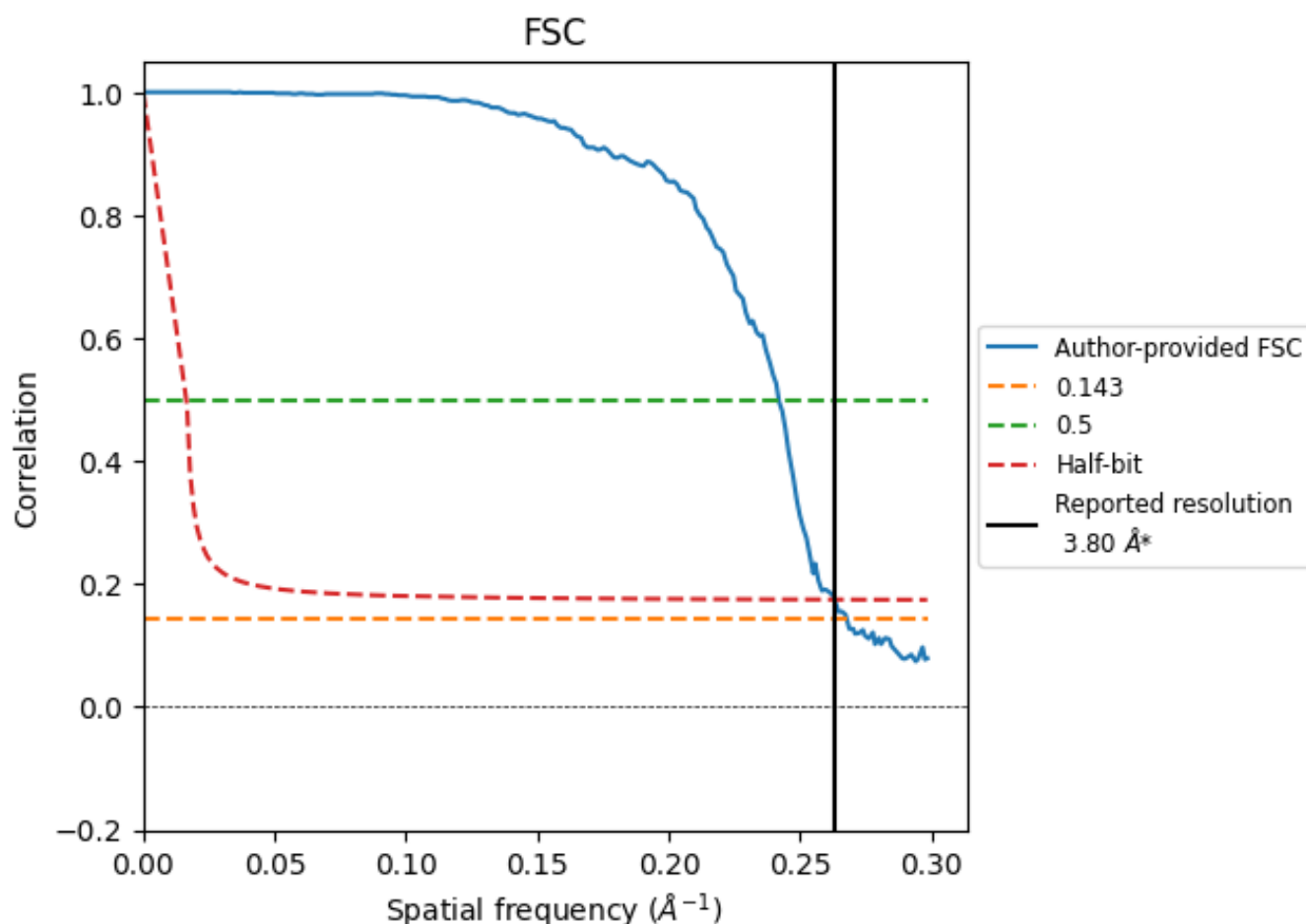


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.73	4.13	3.80
Unmasked-calculated*	-	-	-

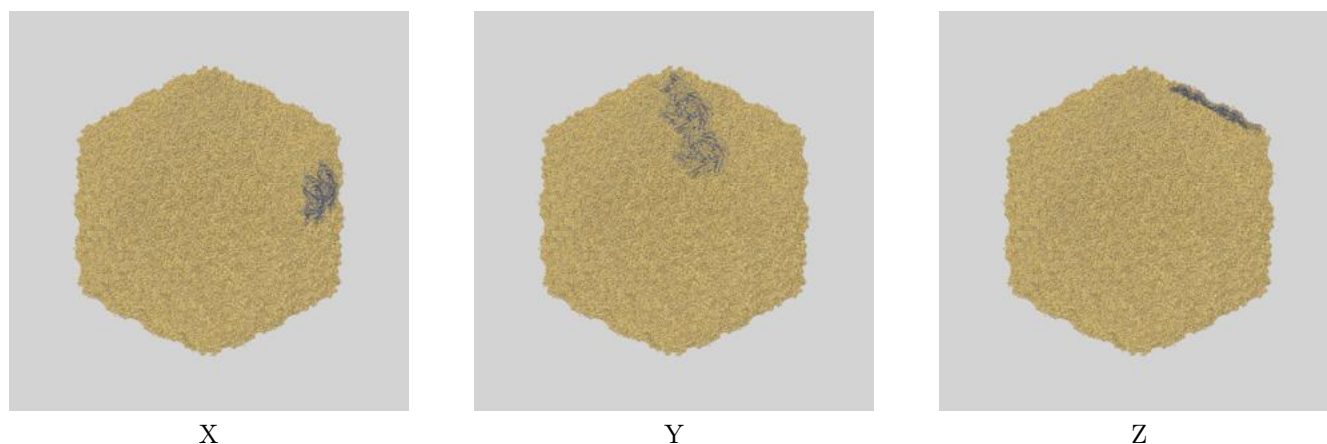
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20125 and PDB model 6OMC. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



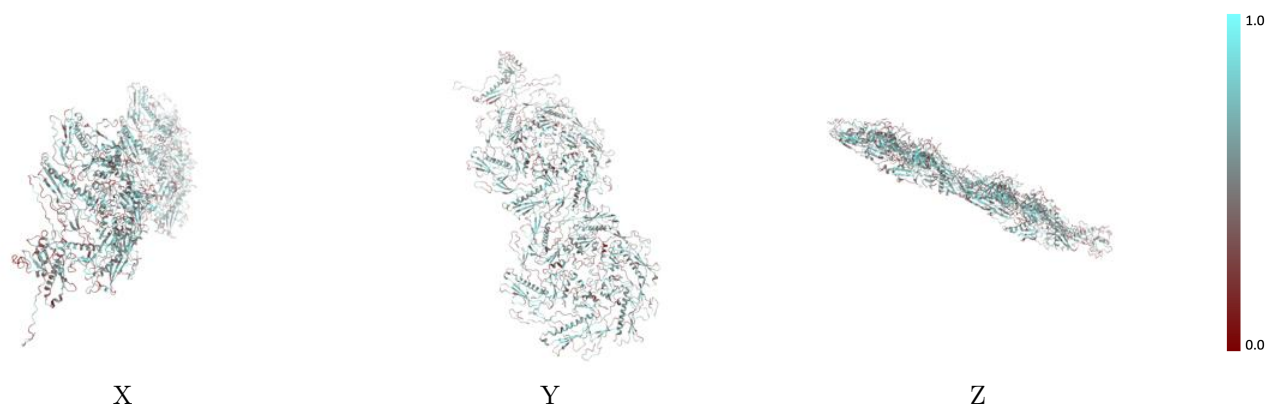
The images above show the 3D surface view of the map at the recommended contour level 8.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



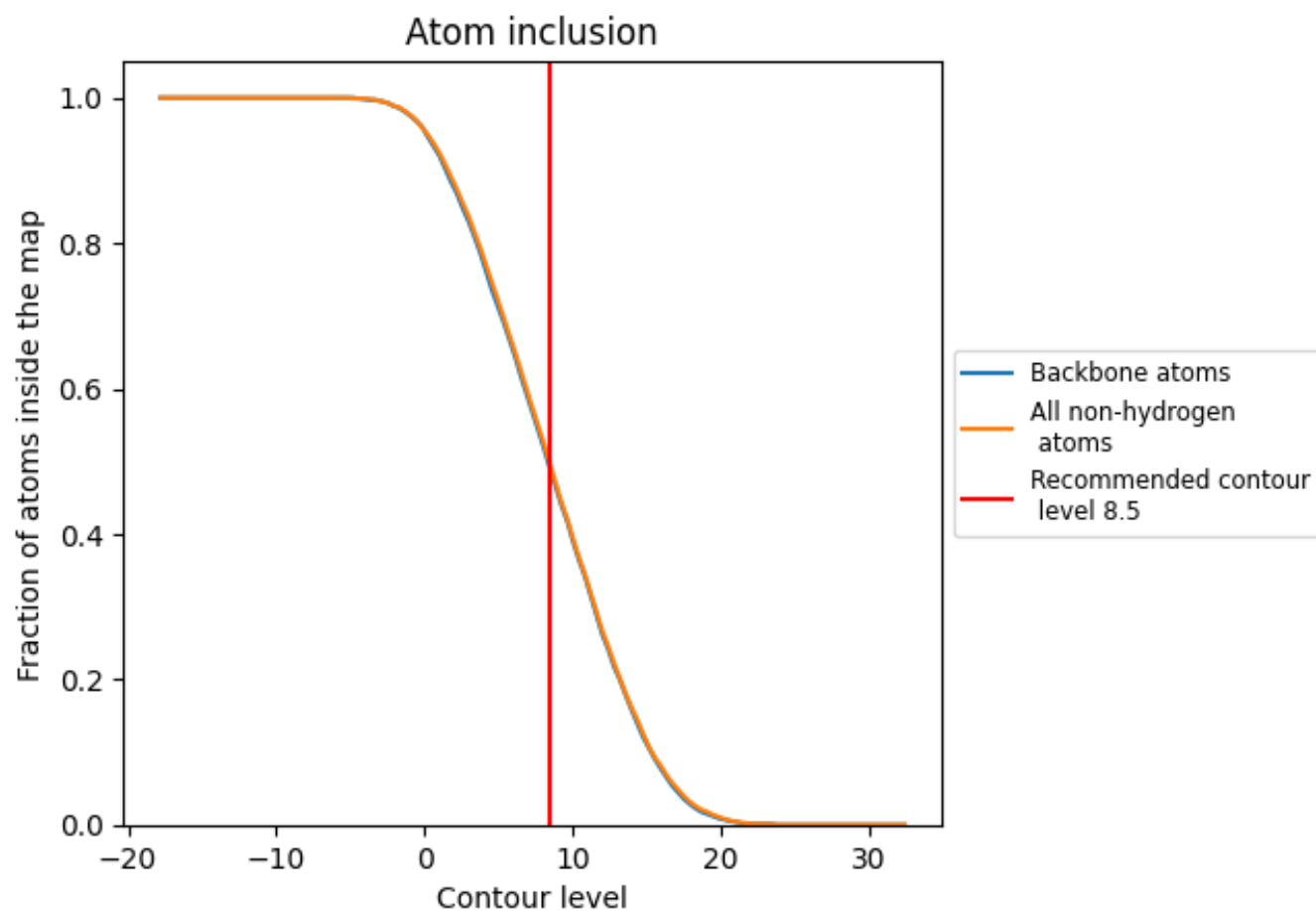
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (8.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4960	0.2770
A	0.5090	0.2790
B	0.5130	0.2810
C	0.5080	0.2690
D	0.5210	0.2690
E	0.5090	0.2660
F	0.5220	0.2790
G	0.4980	0.2730
H	0.5210	0.2800
I	0.5240	0.2790
J	0.5210	0.2890
K	0.4950	0.2840
L	0.4920	0.2840
M	0.4110	0.2650

1.0

0.0

<0.0